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The successive linear estimator: a revisit

J.A. Vargas-Guzmán *, T.-C. Jim Yeh

Department of Hydrology and Water Resources, The University of Arizona, Tucson, AZ 85721, USA

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Abstract

This paper examines the theoretical basis of the successive linear estimator (SLE) that has been developed for the inverse problem in subsurface hydrology. We show that the SLE algorithm is a non-linear iterative estimator to the inverse problem. The weights used in the SLE algorithm are calculated based on conditional covariances, and yield estimates that satisfy the minimum-mean-square-error criterion. Furthermore, the weights for well-posed or deterministic inverse problems are equivalent to the inverse of Jacobian matrices of the classical Newton–Raphson (NR) algorithm for the non-linear forward problem. For ill-posed or stochastic inverse problems, the weights are smooth interpreted quantities of the inverse of the Jacobian at data locations, based on the spatial covariance of parameters. For both deterministic and stochastic inverse problems, the SLE algorithm converges as in the NR scheme for the forward non-linear problem.

The SLE approach is verified with a simple forward exponential model and compared to the exact lognormal conditional mean estimates. Results show that for the deterministic inverse problem, this approach can yield an exact solution, whereas the estimate of the SLE approach for the stochastic inverse problem is exact up to a known residual term related to the conditional estimation variance.

Keywords: Inverse problem; Cokriging; Non-Gaussian random fields; Non-linear model; Conditional mean

1. Introduction

Characterizing the spatial distribution of hydraulic properties of porous media is a necessary step towards high-resolution predictions of water flow and contaminant transport in an aquifer. High-density measurements of hydraulic properties over a large volume of an aquifer are rare, cost-prohibitive and practically impossible. Measurements of responses of an aquifer, on the other hand, are generally less costly and abundant. Making use of the abundant measurements of an aquifer's responses to characterize the spatial distribution of its hydraulic properties is therefore a logical step. This is known as the inverse problem in subsurface hydrology.

Numerous researchers have developed various methods to solve the inverse problem during the last few decades. Most of these methods use sparsely monitored hydraulic head $\phi(x)$, to derive the spatially distributed transmissivity $T(x)$, that minimizes an objective function, $\sum(\phi(x) - \hat{\phi}(x))^2$, where $\hat{\phi}(x)$ is the simulated head based on the estimated transmissivity $\widehat{T}(x)$. The method is, generally, a least-squares optimization approach with some variations. See [2,17,18] for a comprehensive review of the methods.

The other approach that has become popular during the past decade is the geostatistically based approach, cokriging (e.g., [4–6,8–10,13,16,20,22,23,25]). For a mildly heterogeneous aquifer, where the perturbation of the natural logarithm of the transmissivity is linearly related to the perturbation of the hydraulic head field, it can be shown that cokriging and classical optimization approaches yield identical solutions. This is true if the least-squares optimization approach starts with kriged parameter estimates and considers the spatial covariance of the parameter [14,3]. Cokriging nevertheless differs from the least-squares approach in many ways. The least-squares approach is a regression model that considers only the sensitivity matrix (i.e., model cross-correlation structure) of the model response to changes in the parameter. Conversely, cokriging is a linear estimator based on observations, and it uses: the spatial covariance of the parameter; the spatial covariance of the response of the model; the spatial cross-covariance of the parameter; and the response to yield the estimate

* Corresponding author.

E-mail addresses: a.varguz@mailbox.uq.edu.au (J.A. Vargas-Guzmán), yeh@hwr.arizona.edu (T.-C.J. Yeh).

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that satisfies the minimum-mean-square-error criterion. Unlike the sensitivity matrix, the spatial cross-covariance is a product of the spatial covariance of the parameter and the sensitivity matrix.

Computational algorithms of the two approaches are also different. Cokriging estimates a parameter at one location at a time using all the observations simultaneously or sequentially [19], although simultaneous estimation of parameters at all locations is possible [15]. On the other hand, the classical least-squares approach generally requires estimation of parameters at all locations using all available observations simultaneously.

It is a well-known fact that cokriging implicitly assumes the stochastic parameter is a Gaussian process [15]. Whether or not the process is Gaussian, the argument is that if the process is Gaussian, then cokriging is the best linear unbiased estimator; if the process is non-Gaussian, cokriging gives merely a best "linear" predictor.

Cokriging is a linear estimator (i.e., it assumes that the transmissivity estimate is a linear combination of the hydraulic head data values) while the relation between the transmissivity and the hydraulic head field in the governing groundwater flow model is non-linear. Therefore, cokriging typically cannot take full advantage of the head information during the estimation. To overcome this limitation of the classical cokriging method, Yeh et al. [24] developed a successive linear estimator (SLE) approach. The approach is similar to that developed by Gutjahr et al. [7], but the SLE method considers the successive improvement of the conditional covariance.

While cokriging estimates the conditional mean of the transmissivity and the hydraulic head in a Gaussian framework, the SLE method estimates the conditional effective transmissivity and hydraulic heads. To illustrate this difference, consider the case of steady flow in the aquifer that is described by the governing groundwater flow equation:

$$\nabla \cdot [T(x)\nabla\phi(x)] = 0 \tag{1}$$

which is subject to some given boundary conditions. In Eq. (1), x denotes the coordinates, T is the parameter (transmissivity), and ϕ is the response (the hydraulic head) of the system. To derive the inverse solution to Eq. (1) with sparse measurements of the hydraulic head and the transmissivity, Yeh et al. [24] resort to the conditional stochastic representation. That is, they considered possible solutions (transmissivity fields) to the inverse problem as realizations of a stochastic process that are conditioned to observations. Each conditional realization of the transmissivity field can thus be expressed as the sum of the conditional expected value, $E[]$, and a perturbation, i.e., $\ln T(x) = E[\ln T(x)] + \tau(x)$, where ln is the natural logarithm. Because of the stochastic representation, the hydraulic head also is considered as a stochastic process conditioned on the observation and thus $\phi(x) = E[\phi(x)] + h(x)$. Replacing the transmissivity and the hydraulic head in Eq. (1) with the stochastic process, and taking the expected value of Eq. (1), one derives a conditional-mean-flow equation:

$$\begin{aligned}&\left[\nabla^2 E[\phi(x)] + \nabla E[\ln T(x)] \cdot \nabla E[\phi(x)]\right] \\ &\quad + E[\nabla[\tau(x)] \cdot \nabla[h(x)]] = 0\end{aligned} \tag{2}$$

As indicated in Eq. (2), the conditional mean transmissivity and head fields do not satisfy mass balance unless the second term is zero. The term will be zero only if no uncertainty exists in the hydraulic head or the transmissivity field, and boundary conditions and the flux are known exactly. Otherwise, this term $E[\nabla[\tau(x)] \cdot \nabla[h(x)]]$ must be determined a priori; however, evaluation of this term is usually intractable. Consequently, Yeh et al. [24] resort to the use of a conditional effective transmissivity $T_{\text{ceff}}(x)$ and head $\phi_{\text{ceff}}(x)$ fields that satisfy the mass balance requirement, i.e., $\nabla \cdot [T_{\text{ceff}}(x)\nabla\phi_{\text{ceff}}(x)] = 0$. In other words, the contribution of the second term is distributed to both T_{ceff} and ϕ_{ceff}. According to this approach, the conditional effective transmissivity is a parameter field that agrees with the transmissivity measurements at sample locations. Moreover, it yields a conditional effective hydraulic head field that preserves values of the hydraulic head measurements when it is used in Eq. (1).

Parallel to the SLE method, Vargas-Guzmán and Yeh [19] developed the theory of sequential kriging and cokriging. In sequential kriging, the difference between the observed value and the estimate, and the sequential update of the conditional covariance function are used to obtain the updated estimate. While the algorithm and procedure of the SLE for the inverse problem and sequential kriging are similar, the goals of the two are different. Sequential kriging splits a large data set into subsets, and each subset is included sequentially in the estimation. Conversely, SLE successively incorporates the non-linear effect into estimation of model parameters. For a linear system, Vargas-Guzmán and Yeh [19] showed that sequential kriging is identical to kriging using all the data sets simultaneously.

While many hydrological applications of the SLE method to hydrological problems (e.g., [11,21,24,25]) have demonstrated the robustness of the method, its convergence and properties of the estimated conditional effective parameters remain to be examined. The objective of this study is to visit the theoretical basis of the convergence of the SLE method and to verify the estimate of the SLE method by using a simplified non-linear model. The simplified model relates two random fields through an exponential relation, which can be linearlized after a logarithm transformation. Therefore, the exact conditional mean can be derived using classical lognormal kriging. The difference between the estimate

by the SLE method and the exact conditional mean is subsequently analyzed.

2. Review of successive linear estimator

2.1. A non-linear estimator

To account for non-linearity between the response (the hydraulic head) and the parameter (the transmissivity) of a system (the aquifer), the SLE method starts with an initial cokriging estimate $\widehat{T}^1(x)$ at each location in the domain (see [24] for details). Subsequently, a forward model for the system (i.e., Eq. (1)) is solved using $\widehat{T}^1(x)$ for $\hat{\phi}(x)$ and the vector of errors $\Delta\phi(x_\beta)$ is computed as

$$\Delta\phi^r(x_\beta) = (\phi(x_\beta) - \hat{\phi}^r(x_\beta)) \tag{3}$$

where the superscript r is the iteration index, $\phi(x_\beta)$ is a vector of n observed responses at the sample locations $\{x_\beta|\beta = 1,\ldots,n\}$, and $\hat{\phi}^r(x_\beta)$ is the vector of the response at sample locations x_β computed from the forward model. The updated parameter estimate $\widehat{T}^{r+1}(x)$ at any iteration $r+1$ is:

$$\widehat{T}^{r+1}(x) = \widehat{T}^r(x) + \varpi^{\mathrm{T}}\Delta\phi^r(x_\beta) \tag{4}$$

Note that hereafter a superscript T means transpose unless otherwise indicated. The transpose of the vector of weights ϖ^{T} for Eq. (4) is obtained by solving a system of equations at each step. That is,

$$\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta\phi}\varpi = \boldsymbol{\varepsilon}^r_{\Delta\phi\Delta T} \tag{5}$$

where $\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta\phi}$ and $\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta T}$ are the conditional (or residual) covariance and cross-covariance of the residuals $\Delta\phi$ and ΔT and $\Delta T = \widehat{T}^{r+1} - \widehat{T}^r$. Calculations of the covariance and cross-covariance are discussed in Section 2.2.

The system of Eq. (5) for the residuals may be ill conditioned during iterations and the solution can be unstable. Consequently, a stabilizer is added to the major diagonal of $\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta\phi}$. The procedure (Eqs. (3)–(5)) iterates until the variance of estimated parameters convergences [11,21,24,25].

2.2. First-order approximation for covariances

In order to evaluate the weights in Eq. (5), the covariance of the residual parameter, $\boldsymbol{\varepsilon}^r_{\Delta T\Delta T}$, and the error response attribute, $\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta\phi}$, and the cross-covariance between the parameter and response residuals, $\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta T}$, must be specified [24]. While $\boldsymbol{\varepsilon}^r_{\Delta T\Delta T}$ is specified a priori, both $\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta\phi}$ and $\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta T}$ are approximated using the first-order approximation approach as follows:

$$\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta T} = \mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T} \tag{6}$$

$$\boldsymbol{\varepsilon}^r_{\Delta\phi\Delta\phi} = \mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T}\mathbf{J}^{\mathrm{T}} \tag{7}$$

where $\mathbf{J}$ is the Jacobian or sensitivity matrix of the forward model. The residual covariance $\boldsymbol{\varepsilon}^r_{\Delta T\Delta T}$ is computed at each iteration as

$$\boldsymbol{\varepsilon}^{r+1}_{\Delta T\Delta T} = \boldsymbol{\varepsilon}^r_{\Delta T\Delta T} - (\varpi^r)^{\mathrm{T}}\boldsymbol{\varepsilon}^r_{\Delta T\Delta\phi} \tag{8}$$

Notice that for $r = 2$ the residual covariances may be computed including the weights $\boldsymbol{\lambda}$ for the few m data parameters $T(x_\alpha)$ available at locations $\{x_\alpha|\alpha = 1,\ldots,m\}$, where α is the location index where the parameter is observed. That is,

$$\boldsymbol{\varepsilon}^2_{\Delta T\Delta T} = \mathbf{c}_{\Delta T\Delta T} - (\varpi^1)^{\mathrm{T}}\mathbf{c}_{\Delta T\Delta\phi} - \boldsymbol{\lambda}^{\mathrm{T}}\mathbf{c}_{\Delta T\Delta T_\alpha}$$

where $\mathbf{c}_{\Delta T\Delta T_\alpha}$ is the matrix of unconditional covariance for the parameter, and $\mathbf{c}_{\Delta T\Delta\phi}$ is the matrix of unconditional cross-covariance for the parameter and the response.

3. Properties of the successive linear estimator

3.1. The deterministic inversion problem

If the SLE approach described above is applied to a well-posed inverse problem or deterministic problem, it is equivalent to the Newton–Raphson (NR) algorithm. In the case for our discussion, a well-posed problem implies that all the responses within the domain are completely specified at all locations, and are error free. In addition, boundary conditions and fluxes (for groundwater problems) are known.

Substituting the first order approximation (i.e., Eqs. (6) and (7)) into the system of Eq. (5), assuming $\Delta\phi^r$ is known in the entire domain yields

$$[\mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T}\mathbf{J}^{\mathrm{T}}]\varpi = \mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T} \tag{9}$$

Note that in this inverse problem, the number of response data locations $n = N$ and the number of estimated parameter locations N are the same, and $\mathbf{J}$ is a $N \times N$ square matrix for this section. The matrix of weights for the locations to be estimated is then

$$\varpi = [\mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T}\mathbf{J}^{\mathrm{T}}]^{-1}[\mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T}] \tag{10}$$

Rearranging the product (with parenthesis) yields

$$\varpi = [(\mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T})(\mathbf{J}^{\mathrm{T}})]^{-1}[\mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T}] \tag{11}$$

Introducing the inverse operator results in

$$\varpi = (\mathbf{J}^{\mathrm{T}})^{-1}(\mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T})^{-1}[\mathbf{J}\boldsymbol{\varepsilon}^r_{\Delta T\Delta T}] \tag{12}$$

Thus, the square matrices of covariances cancel out and this yields

$$\varpi^{\mathrm{T}} = \mathbf{J}^{-1} \tag{13}$$

The SLE estimator becomes

$$\Delta\widehat{T}^{r+1}(x) = \mathbf{J}^{-1}\Delta\phi(x)^r \tag{14}$$

Eq. (14) shows that the SLE approach for a deterministic inverse problem is analogous to the NR iteration

scheme for solving a non-linear forward problem. In this case, the response attribute is known at all elements in the domain, and no interpolation is required. This special case shows the equivalence between sensitivity matrices and the weights in the SLE. Therefore, the SLE is a non-linear solution technique for the inverse problem. Also notice that in the case of a linear problem, no iterations are required and the approach reduces to simple cokriging.

3.2. The stochastic inverse problem

Consider the stochastic inverse problem where information about the system response is incomplete. If we assume that residuals for the parameter $\Delta\widehat{T}^{r+1}(x_\beta)$ are available at locations of response attributes for direct estimation, then a simple kriging of the residuals would apply such that the entire domain D is directly estimated at each iteration step. That is

$$\Delta\widehat{T}^{r+1}(x) = \left[(\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_\beta})^{-1}\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_D}\right]^{\mathrm{T}}\Delta T^{r+1}(x_\beta) \tag{15}$$

where $\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_\beta}$ and $\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_D}$ represent the covariance between the parameter residuals at sample locations, and the covariance between the parameter residuals at sample locations and all other locations in the domain, respectively. For the stochastic inverse problem, the estimator is

$$\Delta\widehat{T}^{r+1}(x) = \boldsymbol{\varpi}^{\mathrm{T}}\Delta\phi^r(x_\beta) \tag{16}$$

Combining both Eqs. (15) and (16), one obtains

$$\left[(\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_\beta})^{-1}\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_D}\right]^{\mathrm{T}}\Delta T^{r+1}(x_\beta) = \boldsymbol{\varpi}^{\mathrm{T}}\Delta\phi^r(x_\beta) \tag{17}$$

For the general case of incomplete response information, consider a reduced square Jacobian matrix $\mathbf{J}_\beta$ for sample locations such that

$$\Delta\widehat{T}^{r+1}(x_\beta) = \mathbf{J}_\beta^{-1}\Delta\phi^r(x_\beta) \tag{18}$$

Note that the terms $\Delta\widehat{T}^{r+1}(x_\beta)$ and $\Delta\phi^r(x_\beta)$ appear in both Eqs. (17) and (18). Multiplying Eq. (17) by the transpose vector $(\Delta\phi^r(x_\beta))^{\mathrm{T}}$ gives

$$\left[(\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_\beta})^{-1}\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_D}\right]^{\mathrm{T}}\Delta T^{r+1}(x_\beta)(\Delta\phi^r(x_\beta))^{\mathrm{T}} = \boldsymbol{\varpi}^{\mathrm{T}}\Delta\phi^r(x_\beta)(\Delta\phi^r(x_\beta))^{\mathrm{T}} \tag{19}$$

The same operation for Eq. (18) is

$$\Delta\widehat{T}^{r+1}(x_\beta)(\Delta\phi^r(x_\beta))^{\mathrm{T}} = \mathbf{J}_\beta^{-1}\Delta\phi^r(x_\beta)(\Delta\phi^r(x_\beta))^{\mathrm{T}} \tag{20}$$

After rearranging Eq. (19) by leaving the weights on the right-hand side, Eq. (19) becomes

$$\left[(\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_\beta})^{-1}\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_D}\right]^{\mathrm{T}}\Delta T^{r+1}(x_\beta) \times (\Delta\phi^r(x_\beta))^{\mathrm{T}}\left[\Delta\phi^r(x_\beta)(\Delta\phi^r(x_\beta))^{\mathrm{T}}\right]^{-1} = \boldsymbol{\varpi}^{\mathrm{T}} \tag{21}$$

Applying the same operation to Eq. (20) gives

$$\Delta\widehat{T}^{r+1}(x_\beta)(\Delta\phi^r(x_\beta))^{\mathrm{T}}\left[\Delta\phi^r(x_\beta)(\Delta\phi^r(x_\beta))^{\mathrm{T}}\right]^{-1} = \mathbf{J}_\beta^{-1} \tag{22}$$

Eq. (22) is analogous to the cokriging system. Notice that the vectors of products give square matrices of second moments for the Jacobians. Substituting Eq. (22) into Eq. (21) yields

$$\left[(\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_\beta})^{-1}\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_D}\right]^{\mathrm{T}}\mathbf{J}_\beta^{-1} = \boldsymbol{\varpi}^{\mathrm{T}} \tag{23}$$

This shows that the SLE weights $\boldsymbol{\varpi}^{\mathrm{T}}$ merely are interpolated values of the inverse of the Jacobians $\mathbf{J}_\beta$ at data locations, and Eq. (23) is a simple kriging. The kriging weights $\boldsymbol{\lambda}^{\mathrm{T}}$ for estimation of the SLE weights $\boldsymbol{\varpi}^{\mathrm{T}}$ are $\boldsymbol{\lambda}^{\mathrm{T}} = [(\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_\beta})^{-1}\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_D}]^{\mathrm{T}}$. Thus, the variance of the inverse of the Jacobians at a given step is $\mathrm{var}[\mathbf{J}_\beta^{-1}] - \sigma_{\mathrm{k}}^2(x)$, where $\sigma_{\mathrm{k}}^2(x) = [\boldsymbol{\varepsilon}^{r+1}_{\Delta T_\beta \Delta T_D}]^{\mathrm{T}}\boldsymbol{\lambda}$ is the kriging variance. This is coherent with the smoothing effect of kriging [19], where a small kriging variance reflects the impact of information. In the extreme case of complete response information, the estimation variance of the inverse of the Jacobian is zero everywhere, and weights equal the inverse of the Jacobians for the deterministic NR scheme. However, the weights $\boldsymbol{\lambda}^{\mathrm{T}}$ change for each iteration of the SLE procedure, in a manner similar to the modification of the Jacobian at each iteration in the classical NR scheme for solving the non-linear forward problem.

Notice also that the smoothing effect for estimated parameters is different. The smoothness of estimated parameters is caused by: (1) uncertainty at unsampled locations; and (2) the linear approximation of the non-linear relation between perturbations of the parameter and the response of the system. The former diminishes if more information is included in the estimation, while the latter will reduce only through iterations to account for the non-linearity. The cokriging parameter estimation variance can be quantified for each iteration from the cokriging weights multiplied by the right-hand side cross-covariances in Eq. (9). Then, using Eq. (23), the estimation variance for a single step is $\sigma_{\mathrm{k}T}^2 = [\mathbf{J}\boldsymbol{\varepsilon}^{r+1}_{\Delta T_D \Delta T_D}]^{\mathrm{T}}[\boldsymbol{\lambda}^{\mathrm{T}}\mathbf{J}_\beta^{-1}]^{\mathrm{T}}$. In practice, the smoothing effect for parameters will reduce as the solution converges.

3.3. Convergence of the successive linear estimator

Recall the well-known differential mean value theorem [1]. Let a function $\phi(T)$ be continuous for an interval $a \leqslant T \leqslant b$ and differentiable for $a < T < b$; there exists at least one mean value of $T = \widetilde{T}$ for which the approximate Jacobian derivative is exact. This is

$$J_i = \frac{\partial\phi(\widetilde{T})}{\partial\widetilde{T}} = \frac{\phi(b) - \phi(a)}{b - a} \tag{24}$$

The above theorem can be extended for a theoretical inverse of the SLE weights. Considering vectors for the set of data locations, the difference between the true and

the updated response estimate using the SLE estimated parameters at step r is

$$\phi(T) - \hat{\phi}^r(\widehat{T}^r) = \left[[\varpi(T + \xi(\widehat{T}^r - T))]^{-1}\right]^{\mathrm{T}}(\widehat{T}^r - T) \tag{25}$$

where $\varpi(T + \xi(\widehat{T}^r - T))$ is a square matrix that involves only the unknown weights, ϖ, for response data locations, and it should provide estimates of the vector $T = \widetilde{T}$ at x_β sample locations. The parameter ξ is a number between zero and one, and will be closer to one depending on the amount of deviation. These weights will not exactly yield the true residual at a specific step, but they will be exact for some value in the interval between the true and the estimated residual value. Thus, Eq. (25) relates the deviations in an exact way. The iterative updating of parameters is

$$\widehat{T}^{r+1} - T = \widehat{T}^r + \Delta T^{r+1} - T \tag{26}$$

And since one step of the SLE estimator is

$$\Delta T^r = (\varpi^r)^{\mathrm{T}}\Delta\phi^{r-1} \tag{27}$$

Then

$$\Delta T^r = (\varpi^r)^{\mathrm{T}}\left[\left[[\varpi(T + \xi(\widehat{T}^{r-1} - T))]^{-1}\right]^{\mathrm{T}}(\widehat{T}^{r-1} - T)\right] \tag{28}$$

and

$$\Delta T^{r+1} = (\varpi^{r+1})^{\mathrm{T}}\left[\left[[\varpi(T + \xi(\widehat{T}^r - T))]^{-1}\right]^{\mathrm{T}}(\widehat{T}^r - T)\right] \tag{29}$$

If the last step has been achieved, $\widehat{T}^{r+1} \cong T$ and

$$\Delta T^{r+1} = (\psi)^{\mathrm{T}}\left(\left[[\varpi(T + \xi(\widehat{T}^r - T))]^{-1}\right]^{\mathrm{T}}(\widehat{T}^r - T)\right) \tag{30}$$

where the weights ψ provide the ultimate residual to achieve the true T. Following Eq. (26), one has

$$T^{r+1} - T = (\psi)^{\mathrm{T}}\left(\left[[\varpi(T + \xi(\widehat{T}^r - T))]^{-1} - [\psi(T + \xi(\widehat{T}^r - T))]^{-1}\right]^{\mathrm{T}}(\widehat{T}^r - T)\right) \tag{31}$$

Thus, to achieve $|T^{r+1} - T| \leqslant |\widehat{T}^r - T|$ the condition is

$$0 \leqslant \psi^{\mathrm{T}}[\varpi^{-1} - \psi^{-1}]^{\mathrm{T}} \leqslant \mathbf{1} \tag{32}$$

where $\mathbf{1}$ is the vector of unity; this guarantees that $\lim_{r\to\infty}|\Delta T^r| \to 0$, because each term in the positive definite matrix of weights may be kept $\psi_{ij} \leqslant \varpi_{ij}$ for each row-column location, (i, j). This last statement shows the convergence, and it is extended to non-linear interpolation because the non-collocated weights involving non-data locations are smooth versions of the weights involved in the proof. For the deterministic case, this convergence equals that of the classical NR iteration scheme. This provides a proof of the convergence of the SLE algorithm.

4. Verification of successive linear estimator

4.1. The exponential forward model

It is difficult to verify the SLE approach for inverse problems of subsurface hydrology associated with sparse hydraulic head data because the relationship between the parameter and response of the system is nonlinear and the exact conditional mean is difficult to obtain. Consequently, we have to resort to a simplified forward model, which has a known inverse solution. The simplified forward model is:

$$\phi(x) = \exp(aT(x)) \tag{33}$$

where $T(x)$, the parameter (i.e., the transmissivity), has a Gaussian probability density function (pdf), and $\phi(x)$, the response (i.e., the hydraulic head), has a skewed lognormal pdf, and a is a constant parameter. Note that flow models based on Eq. (1) will yield a response-parameter relation that involves convolutions. Logarithmic linearization of Eq. (33) gives a model analogous to a linear filter in the Hilbert space. Note that in this example the parameter and response have a collocated correlation. Because of this exponential relation, a log transformation of Eq. (33) leads to a Gaussian model, and the exact conditional mean of $\ln[\phi(x)]$ can be obtained by using kriging or a linear estimator. On the other hand, the exponential relation between $\phi(x)$ and $T(x)$ provides a test of the ability of SLE to obtain conditional mean estimates $\widehat{T}(x)$ from samples of $\phi(x_\beta)$ which produce the optimum output $\hat{\phi}(x)$. If our SLE method is a non-linear estimator, it should yield the identical results as those derived from the linearized approach.

4.2. The lognormal kriging

Estimating $\hat{\phi}(x_0)$ for the conditional mean at non-sample locations based on $\widehat{T}(x)$ using simple kriging, a linear estimator, is not optimal because of the non-linearity between $T(x)$ and $\phi(x)$, as shown in Eq. (32). However, a log tranformation yields a linear relationship:

$$aT(x_\beta) = \log(\phi(x_\beta)) \tag{34}$$

The data vector $\phi(x_\beta)$ at locations $(x_\beta|\beta = 1, \ldots, n)$ of skewed lognormal distributed data is therefore transformed into $\mathbf{T}(x_\beta)$, which is considered to belong to a Gaussian random field $\mathbf{T}(x)$ with covariance matrix $\mathbf{c}_{TT}$. Simple kriging is applied using

$$\mathbf{c}_{TT}\boldsymbol{\lambda}_{TT_0} = \mathbf{c}_{TT_0} \tag{35}$$

The conditional mean estimate is a linear combination of the normalized data [12]. That is

$$\widehat{T}(x_0) = \boldsymbol{\lambda}_{TT_0}^{\mathrm{T}} \mathbf{T}(x_\beta) \tag{36}$$

However, the estimates $\hat{\phi}(x_0)$ must be obtained with a correction term, which for $a = 1$ is half of the simple kriging variance σ_{k}^2. Then,

$$\hat{\phi}(x_0) = \exp\left[a\widehat{T}(x_0) + \frac{a^2\sigma_{\mathrm{k}}^2}{2}\right] \tag{37}$$

The correction term is easily demonstrated by considering that $T(x)$ is Gaussian and $\phi(x)$ is the exponential function:

$$E(\phi|\phi(x_\alpha)) = \int_{-\infty}^{\infty} \exp(aT(x)) \frac{1}{\sigma_{\mathrm{k}}\sqrt{2\pi}} \times \exp\left(-\frac{(T(x) - E[T(x)])^2}{2\sigma_{\mathrm{k}}^2}\right) \mathrm{d}T \tag{38}$$

where σ_{k} represents the conditional standard deviation or root square of the simple kriging variance, and $\widehat{T}(x) \cong E[T(x)]$ is the Gaussian conditional mean. Then, taking the conditional expected value $E[\phi(x)|\phi(x_\alpha)] \cong \hat{\phi}(x)$ by completion of squares of the exponents yields the same result as Eq. (37).

4.3. Successive linear estimator for the exponential model

To solve the inverse problem with the SLE method, the attributes related by the exponential model are split into mean and perturbation components. Introducing these terms into the forward model, Eq. (33), gives

$$E[\phi(x)] + h(x) = \exp a(E[T(x)] + t(x)) \tag{39}$$

The inverse problem intends to estimate $\widehat{T}(x) \cong E[T(x)]$ from response data. The covariance structure $\mathbf{c}_{\Delta T\Delta T}$ for the parameters of the perturbation of model is known a priori. The first-order approximation approach is used to compute the covariances and cross-covariance matrices required in the SLE approach, as explained previously. The sensitivity matrix for this particular problem is a diagonal matrix where the elements are computed as

$$\frac{\partial\phi(x)}{\partial T(x)} = a\exp(aT(x)) \tag{40}$$

where $a = 1$ for the classical lognormal case. The covariances $\mathbf{c}_{\Delta\phi\Delta\phi}$ and cross-covariances $\mathbf{c}_{\Delta\phi\Delta T}$ are computed iteratively with the first-order approximation, and $\mathbf{c}_{\Delta T\Delta T}$ are from a exponential covariance model.

4.4. The residual term in the exponential model

Taking the expected value of the forward exponential model and considering $E[h(x)] = 0$ yields

$$E[\phi(x)] = \exp(aE[T(x)])E[\exp(at(x))] \tag{41}$$

Notice the "residual" term $E[\exp(at(x))]$ is the conditional expected value of an exponential function of the perturbation of the parameter, which is conditioned to the information of the response attribute. If this expected value is considered conditional to the information of the response attribute, and if the parameter information is Gaussian, $E[\exp(at(x))]$ corresponds to the case computed above. We already know that for lognormal kriging, the expected value is one half of the kriging variance. However, following the classical approach, we do not include this term in the iterative SLE approach, because we want to test the algorithm in the same way as it was used in the inverse problem with flow models, where the residual terms can not be easily predicted. Therefore, we may resort to the use of "effective" mean parameters [24]. That is, $E(\phi) = \exp\{aE[T(x)]_{\mathrm{eff}}\}$.

4.5. Experimental results for the exponential model

In this experiment, we use a domain consisting of 120 elements, in one dimension, and only seven of them correspond to a sample of non-Gaussian response data $\phi(x_\beta)$ at locations $(x_\beta|\beta = 1,\ldots,7)$ located at regular spacing intervals of 20 m. The mean of the parameters $E[T(x)]$ is independent of location and the unconditional mean of the response attribute is $E[\phi(x)]$, which is a function of location representing the mean steady state hydraulic head. For our example of the exponential model used here, stationarity of the parameter's random field implies stationarity of the response random field attribute. However, the stationarity assumption is not required for the SLE non-stationary processes merely increase the variance within the size of the domain and thus the non-linearity of the problem. The covariance for the parameter attribute is assumed to be exponential with a correlation range of 50 and a sill of 1 with arbitrary units.

Note that the exponential forward model in Eq. (39) was used without considering the conditional mean model to make the problem equivalent to the setup of the hydrological mean flow models where residual terms are ignored and exact conditional mean equations are not used.

For comparison purposes, the parameter attribute has been first estimated by lognormal kriging as explained above. Then, using a FORTRAN program coded with the SLE approach, the parameter and response attributes were estimated at all 120 locations. A stabilizer was empiricaly found to equal 0.017 in this particular case. The iteration stops when the L2 norm, $\sum(\phi(x) - \hat{\phi}(x))^2$, and variance of the estimates dropped to specified values.

Fig. 1 shows the estimated values from the SLE method and lognormal simple kriging for the parameter attribute $\widehat{T}(x)$ where the intersection points correspond to sample locations at location (0, 20, 40, 60, 80, 100 and

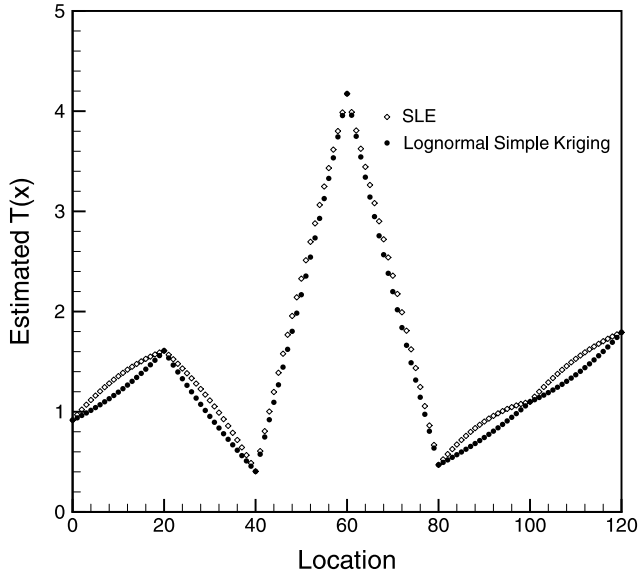

Fig. 1. Parameters estimated with the SLE and lognormal approaches.

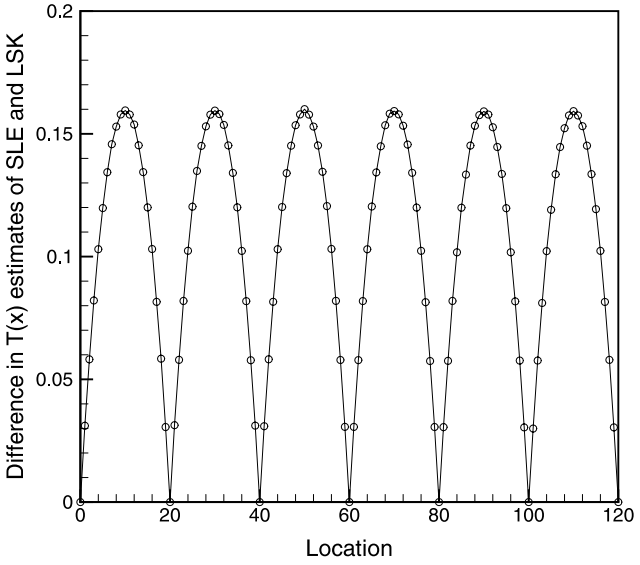

Fig. 3. Deviations of the SLE parameter estimates from the true parameter values.

120). The SLE approach apparently overestimates the conditional estimates $\widehat{T}(x)$ for the parameter attribute. Fig. 2 is a scatter plot of the estimates $\widehat{T}(x)$ from the SLE algorithm versus those of simple kriging using log-transformed response data. It shows that the SLE algorithm overestimates the values compared to log-normal kriging, which is the known conditional mean for the parameter attribute.

Differences between the estimates $\widehat{T}(x)$ from SLE and the estimates from log transformed data yield the deviations between these two approaches. A plot of these differences at all locations is shown in Fig. 3. Surprisingly, the differences show up as deterministic arcs, which were unclear in Fig. 2 because of the presence of the slope. They are not random and in fact are related to the relative location with respect to the samples.

To provide an explanation of these arcs of deviations, Fig. 4 shows a plot of the error or difference in the estimates for the 120 elements in the domain versus the classical kriging variance of the simple kriging of the parameter information. A regression analysis shows a coefficient of determination of 0.999 and a slope equal to 0.5. The deviations are half of the kriging variance as usually utilized in lognormal kriging (see Eq. (36)). This result demonstrates the ability of the SLE algorithm to iteratively perform non-Gaussian (lognormal)

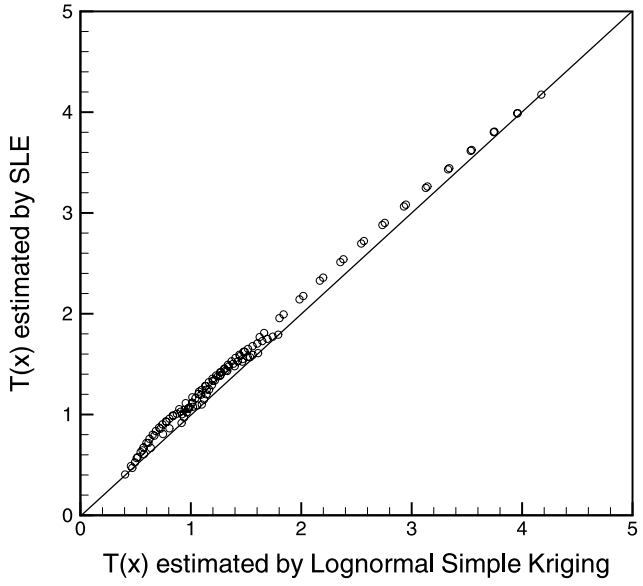

Fig. 2. A scatter plot of the parameter estimates by the SLE versus lognormal simple kriging.

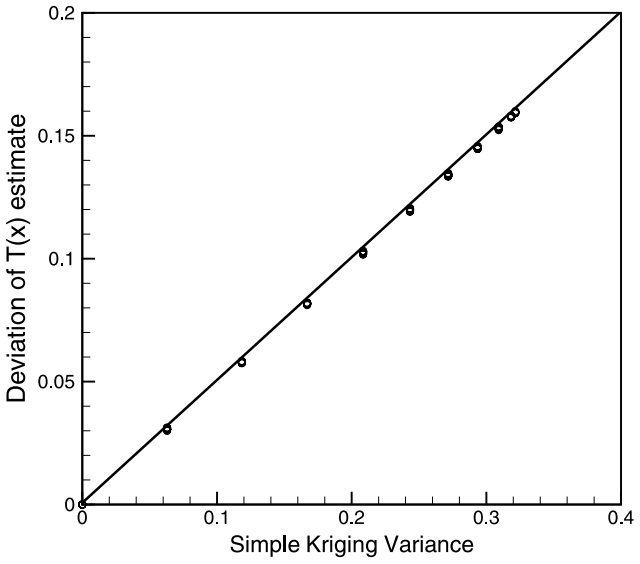

Fig. 4. Linear regression of kriging variances versus the deviations.

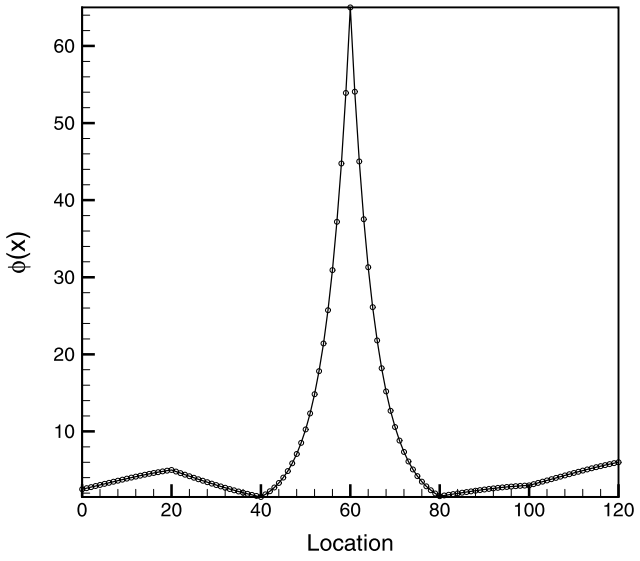

Fig. 5. Non-Gaussian response estimated with the SLE approach (symbol) and lognormal simple kriging (line).

geostatistical estimations and solve the inverse problem. This result, plus the previous theoretical analysis, demonstrates that the SLE algorithm is a non-linear conditional mean estimator up to residual terms.

Finally, Fig. 5 shows that the estimates of response information $\hat{\phi}(x)$ obtained from the SLE are the same as those obtained from the back-transformed lognormal kriging with Eq. (37) plus the mean. This result is expected, given our understanding of the convergence property. Notice that correct results are obtained even though the conditional mean model (i.e., model with conditional residual terms) is not used. Thus, the approach with the exponential model gives the same results as lognormal kriging for the response attribute.

5. Discussion and conclusion

This study has shown through a simplified example and a mathematical analysis that the SLE yields *unique* parameter estimates for a given response data set—different from the classical optimization approach. The SLE predicts the conditional mean of the parameter field up to an *exact* deviation due to residual terms in the mean forward flow model. The role of residual terms in the solution of the inverse problem is non-trivial and may lead to systematic bias in the parameter estimates. Furthermore, the unbiased estimate of the response head converges to the conditional mean that is non-Gaussian. For the lognormal experiment, the residual term coincides with half of the kriging variance, as it is commonly used in lognormal kriging. Thus, the solution of the inverse problem with the SLE is an *unbiased* exact estimate if the residual terms are included into the forward model. The residual terms are a common feature of the expected value of non-Gaussian random variables.

The analysis of both deterministic and stochastic inverse problem shows that the SLE approach for the inverse problems is equivalent to the classical NR scheme for solving non-linear forward problems. The weights of SLE for the deterministic inverse problem are the inverse of the Jacobian of the NR scheme whereas for the stochastic inverse problem, they are smooth interpreted quantities of the inverse of the Jacobian at data locations, based on spatial correlation of the parameter. The classical Gauss–Newton approach is a special case of the SLE where the parameter is considered to be spatially independent. While the Gauss–Newton approach can include the spatial covariance of the parameter, the SLE updates the conditional covariance of the parameter to reflect improvements in the estimate at each iteration. Its final estimates, as a result, are expected to be different those from the Gauss–Newton approach. Furthermore, the SLE offers a more computationally efficient algorithm than the Gauss–Newton approach for determining increments for next iteration. In addition, we show that for both deterministic and stochastic inverse problems, the SLE algorithm converges as in the NR scheme for non-linear forward problems.

The deviations in the parameter attribute estimates (as explained in Figs. 1 and 2) are always positive and do not have a zero mean. This confirms that the estimates behave as conditional effective parameters as suggested by Yeh et al. [24] unless the residual term can be determined and included in the inversion. The spatial distribution of the conditional mean estimated transmissivity values will in general have a lower variance (smoothing effect) because of the interpolation. Also, a deviation is expected because of the omission of residual terms in the classical solutions of the inverse problem in subsurface hydrology. Such bias is caused by the non-linearity of the model, and the number of response data sets. As demonstrated in the example, for skewed lognormal distributions, the error corresponds to the half of the estimation variance. The application of the SLE approach to the inverse problem of Eq. (2) provides a systematic bias in the parameter estimates because of the residual term $E[\nabla(\tau(x)) \cdot \nabla(h(x))]$. A geostatistical estimation of this term requires knowledge of the joint density function of the gradients of perturbations.

Finally, we demonstrated that the SLE approach can successfully estimate the conditional first moment of the parameter using successive linear estimation that is constrained by the governing equation for the conditional first moment. A similar approach may be applicable using higher conditional moments. However, this may require the development of the governing equation with higher conditional moments.

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